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T-dependent structural studies of the oxygen ion conductor $\text{Pr}_{1.5}\text{Sr}_{0.5}\text{NiO}_{4+d}$ investigated by single crystal neutron diffraction

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Mixed-ionic electronic conductors (MIEC) offer significant advantages over conventional cathodes especially in the intermediate temperature range for solid oxide fuel cell applications as well as for oxygen sensors. Ruddlesden-Popper type layered oxides which belong to K_2NiF_4 family are of great scientific interest in this field due to the interplay of the variable structure to tune functional properties. Among them, $\text{Pr}_2\text{NiO}_{4+d}$ is a promising candidate as the compound shows the searched high oxygen mobility already at ambient temperature and the oxygen diffusion can be lowered by Sr doping.

Apical oxygen disorder is regarded as the fundamental prerequisite behind the high oxygen diffusion at moderate temperatures which is described by the phonon assisted diffusion mechanism. In this work, we have explored the effect of Sr doping and temperature on apical oxygen dynamics in $\text{Pr}_{1.5}\text{Sr}_{0.5}\text{NiO}_{4+d}$ by single crystal neutron diffraction. Our diffraction measurements at RT revealed a tetragonal crystal structure for $\text{Pr}_{1.5}\text{Sr}_{0.5}\text{NiO}_{4+d}$ when no structural transitions were evidenced up to 800 C [1]. High structural displacement factors were found for equatorial oxygens along the c-axis and for apical oxygens in the ab-plane with respect to the tetragonal unit cell. Anisotropic displacement parameters are almost linearly increasing with temperature. Comparisons of our results with undoped samples [2] show that Sr doping highly reduces the anisotropic movement both for the apical and equatorial oxygen atoms. To describe the oxygen disorder in the anharmonic approximation at different temperatures, the observed neutron scattering density of the averaged structure was also explored using the Maximum Entropy Method (MEM). These results confirm the anharmonic flat square behavior for apical oxygens with the normal parallel to the c-axis at RT. The outer diameter of the flat square almost reaches up to 0.5 Å which is much less than 2 Å observed for $\text{Pr}_2\text{NiO}_{4.25}$ at already RT.

We conclude from the comparison of our observation in $\text{Pr}_{1.5}\text{Sr}_{0.5}\text{NiO}_{4+d}$ with published results from undoped compounds, that the presence of interstitial oxygen atoms at RT is enhancing the diffusion process by providing a shallow diffusion potential for apical oxygens.

[1] Sumit Maity, Temperature dependent oxygen disorder in $\text{Pr}_{2-x}\text{Sr}_x\text{NiO}_{4+d}$ by high resolution single crystal neutron diffraction in HEiDi, Master Thesis TUM (2015).

[2] M. Ceretti et.al; J. Mater. Chem. A, (2015), 3, 21140.

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